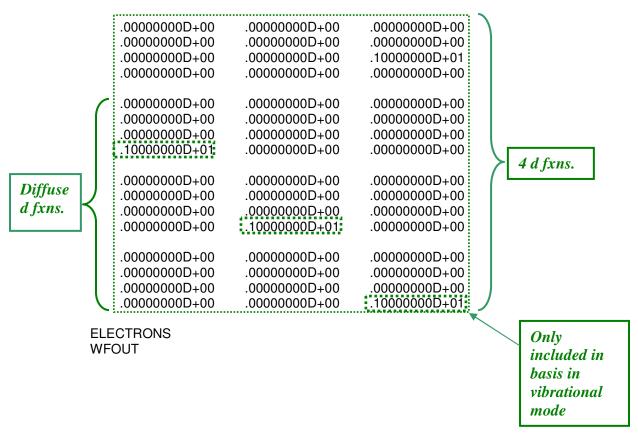
Number of Gaussian primitives in the basis.

These supplementary 1 TOTAL NUMBER OF ATOM TYPES functions are only 6 6 ELECTRONIC AND NUCLEAR CHARGE used in the calculation ALL ALL-ELECTRON ATOM TYPE 1 NUMBER OF ATOMS OF TYPE CAR of vibrational (IR) ALL-CAR001 modes. **EXTRABASIS** CONTROLS USAGE OF SUPPLEMENTARY BASIS FUNCTIONS 12 NUMBER OF BARE GAUSSIANS 3 NUMBER OF S.P.D FUNCTIONS 1 SUPPLEMENTARY S.P.D FUNCTIONS .75790135D+03 22213361D+05 .33317370D+04 $\alpha_1 \alpha_2 \alpha_3$ 21454372D+03 .69924889D+02 .25086135D+02 Gaussian Total number $\alpha_4 \alpha_5 \alpha_6$ 95910418D+01 .38024557D+01 .14891854D+01 exponents of basis .21494732D+00 57487653D+00 .77209650D-01 *Etc* functions of $C_1^l C_2^l C_3^l$ each type is .19792249D+00 .36998977D+00 .63644615D+00 Contraction .14480787D+01 .10124931D+01 .17173689D+01 $C_{4}^{l} C_{5}^{l} C_{6}^{l}$ sum of this coefficients for .68987161D+00 .14931932D+01 .86072247D-01 column. **1st basis fxn.** Etc. -.16566695D-02 .37766033D-03 -.47105343D-04 *This example:* -.45005260D-01 -.84621052D-01 -.14496564D+00 $C_{1}^{2}C_{2}^{2}C_{3}^{2}$ Contraction 5+0=5 s fxns. -.23535601D+00 -.34215368D+00 -.44595124D+00 $C_4^2 C_5^2 C_6^2$ coefficients for -.45263971D+00 -.32216414D+00 -.12988420D-01 4+0 = 4 p fxns. 2^{nd} basis fxn. Etc. .20135471D+00 .12769912D+00 .14135467D-01 3+1=4 d fxns. .0000000D+00 .00000000D+00 .0000000D+00 .0000000D+00 .0000000D+00 .00000000D+00 5 s fxns. .00000000D+00 .0000000D+00 .0000000D+00 .10000000D+01 .0000000D+00 .0000000D+00 .0000000D+00 .0000000D+00 .0000000D+00 .0000000D+00 .0000000D+00 .0000000D+00 Diffuse .0000000D+00 .0000000D+00 .0000000D+00 s fxns. .10000000D+01 .0000000D+00 .10000000D+01 .23138630D-01 .42649133D-01 .74658851D-01 .12024115D+00 .18351176D+00 .24706804D+00 .30714219D+00 .31372706D+00 .26726340D+00 .14756585D+00 .47585576D-01 .72796459D-02 .0000000D+00 .0000000D+00 .00000000D+00 .0000000D+00 .0000000D+00 .0000000D+00 .0000000D+00 .0000000D+00 .0000000D+00 .10000000D+01 .00000000D+00 .00000000D+00 4 p fxns. .0000000D+00 .0000000D+00 .0000000D+00 Diffuse .0000000D+00 .0000000D+00 .00000000D+00 p fxns. .0000000D+00 .0000000D+00 .0000000D+00 .10000000D+01 .0000000D+00 .10000000D+01 .0000000D+00



Basis function Number "N":

$$\phi_{N}(\vec{x}) = \sum_{p=1}^{n_{p}} C_{p}^{N} |\vec{x}|^{l} Y_{lm}(\hat{x}) e^{-\alpha_{p} |\vec{x}|^{2}}$$

where l is the angular moment for basis function N (s,p,d,etc.) and n_p is the number of primitives in the basis (12 in the above example). α_p and C_p^N are the Gaussian exponents and contraction coefficients for basis function N.

In practice a symmetric molecular orbital is the actual basis used in the calculations formed from linear combinations of the above.